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*Research Article*

# Structural Prediction of Bis{(di-*p*-anisole)-1,4-azabutadiene}-bis[triphenylphosphine]ruthenium(II) Using $^{31}$P NMR Spectroscopy

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The present paper reports the use of $^{31}$P NMR spectroscopy to predict the isomer structures of [bis{4-methoxy-phenyl-[3-(4-methoxy-phenyl)-allylidene]-amino}]-bis[triphenylphosphine]ruthenium(II), also known as bis{(di-*p*-anisole)-1,4-azabutadiene}-bis[triphenylphosphine]ruthenium(II), complexes. The complexation reaction was carried out under refluxing condition of (di-*p*-anisole)-1,4-azabutadiene (compound **1**), triphenylphosphine ($PPh_3$), and ruthenium chloride in the ratio of 2 : 2 : 1 for five hours. In addition, ruthenium(II) complexes were also characterized using FTIR and UV-Vis spectroscopy to support the formation of ruthenium(II) complexes. $^{31}$P NMR spectroscopic study on ruthenium(II) complexes suggested that there are three isomers present after the complexation reaction and all the ruthenium complexes demonstrate octahedral geometry.

## 1. Introduction

Nuclear magnetic resonance (NMR) spectroscopy is an essential instrument in chemistry as it can determine the structure of a molecule, the presence of impurities in a sample and the rate of formation as well as degradation of a compound. Even in 1970s, NMR has already been used to determine the cancer formation which offered a simple, fast, and low cost method to identify cancer formation [1–3]. For inorganic chemist, the use of $^{31}$P NMR to identify the structure of a complex containing phosphine ligands is very common [4, 5]. One of the well-known examples is the use of $^{31}$P NMR spectroscopy to determine the Wilkinson hydrogenation mechanism by identifying the coupling patterns among phosphine ligands and also the coupling constants between phosphine ligands as well as rhodium(I) metal centre [6].

In our long term research interest in ruthenium(II) complexes synthesis, we used (di-*p*-anisole)-1,4-azabutadiene (**1**) and triphenylphosphine ($PPh_3$) as the ligands to react with ruthenium trichloride under reflux condition. The products formed were checked by using $^{31}$P NMR spectroscopy and the results found in the spectra are worth to be discussed in the present communication.

## 2. Methodology

The ruthenium complexes were characterized using UV/Vis, FTIR, and $^{31}$P NMR spectroscopy. The IR spectra were recorded using a Thermo Scientific Nicolet iS10 in KBr disc. $^{1}$H NMR spectrum for compound **1** and $^{31}$P NMR spectrum for ruthenium(II) complexes were recorded using JEOL JNM-ECA 500 spectrometer with TMS as an internal standard. The absorption spectra were recorded with Jasco V-630 spectrophotometer.

*2.1. Preparation of (4-Methoxy-phenyl)-[3-(4-methoxy-phenyl)-allylidene]-amine or (di-p-Anisole)-1,4-azabutadiene (**1**).* 4-Methoxycinnamaldehyde (1.62 g, 10.00 mmol) was dissolved in 10 mL of ethanol and followed by 4-methoxyaniline (1.23 g, 10.00 mmol) which was then added to the solution. The reaction mixture was stirred for 4 hours and resulted